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## MONTE-CARLO SIMULATIONS OF GAS DISCHARGE SYSTEMS WITH SOME APPLICATION TO $SF_6$

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SUMMARY

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We use the Monte Carlo method to consider the behaviour of an electron swarm released into a Sulphur HexaFluoride gas discharge. The mean energy of the swarm is monitored as a function of time and when the steady state is reached the energy and velocity distributions are calculated. The growth in electron number is also monitored and this is used to determine the stable working field in the gas. The results confirm that the two term Boltzmann equation is adequate for calculating electron energy distribution functions. Keywords: Great Britain. (RH)



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# 1 Introduction

In gas discharges the molecular energy levels are excited by hot electrons which move through the gas at high speed. The efficiency with which light is emitted from these energy levels is mainly determined by two factors. Firstly a molecule in an excited state favours transitions which are allowed by the selection rules[Smith and Thomson(1978)]. Secondly the efficiency with which the excited state is populated is fixed by the function describing how the energy is distributed amongst the free electrons in the discharge. A knowledge of this distribution and the cross-sections of the molecules involved then fixes the excitation rates uniquely. In this report we are concerned with the calculation of this distribution.

There are two well established methods for solving electron transport problems in gas discharge systems. The first involves considering an electron distribution function which describes the behaviour of large numbers of electrons taken as a whole, this results in the Boltzmann transport equation. The second approach considers the individual behaviour of many electrons and maps out their phase space trajectories, the macroscopic observables are then calculated by taking averages over many electron paths. This is the Monte-Carlo approach.

The Boltzmann equation has been solved for the discharge by many authors[Smith and Thomson(1978), Itoh et al.(1988), Johnson et al.(1979)]. This is usually accomplished by neglecting spatial effects and expanding the distribution in terms of the spherical harmonics[Holstein(1946)]. The expansion is usually truncated at the second term (the so called Lorentz approximation) although some authors have included the third term[Itoh et al.(1988)]. The resulting equations are solved in the relaxation time approximation. The algorithms for solution are usually quick, and take 10's of seconds on a serial computer, but the results are approximate.

In this report we consider the Monte-Carlo method which is exact. The Monte-Carlo treats spatial effects properly, and may be used to generate information which is not easily produced by the Boltzmann approach. It is possible to examine the dynamics in the gas and to evaluate the relaxation times which determine how quickly the gas reaches the steady state. The inclusion of magnetic field effects is also achieved by a simple addition to the code. In spite of all these advantages the results from a Monte-Carlo are noisy unless a very large number of electrons are considered in the simulation. As we are ultimately interested in calculating excitation rates for molecular levels it is the high energy electrons which are of interest and these lie in the tail of the distribution, consequently the excitation rates which depend on integrals over the

tail are particularly noisy. As it can take hours to calculate an excitation rate to an accuracy of a few percent on a serial computer we resorted to parallel techniques. The results presented here were calculated on a transputer based parallel computing system.

We divide this report into six sections. In Section Two we consider the influence of the scattering rates on the free flight time of the electron. We follow Rees(1969) and introduce the concept of self-scattering which simplifies the problem dramatically and results in more efficient computer code. In Section Three we describe the details of the scattering event and outline the computer algorithm. In Section Four we present some results for $SF_6$ and these are compared to the results of a Boltzmann calculation[Milsom et al.(1990)]. Sections Five and Six are devoted to the discussion and conclusions.

## 2 Free-Flight Times and Self-Scattering

In the gas each electron moves freely under the applied electric fields until it suffers a collision with a gas atom. The crux of the problem is to determine two things:- the duration of the free flight and the new electron velocity after the collision. In this section we consider the first of the two.

During free flight the electron's velocity changes continuously because of the applied electric field. If $P[\underline{k}(t)]dt$ is the probability that an electron with momentum $\underline{k}$ suffers a collision during the time dt, the probability that an electron which suffered a collision at time t=0 has not yet suffered another collision after time t is,

$$exp\left[-\int_0^t P\left[\underline{k}(t')\right]dt'\right] \quad . \tag{1}$$

The probability $P(t)dt$ that the electron will suffer its next collision during $dt$ around $t$ is given by

$$P(t)dt = P\left[\underline{k}(t)\right] exp\left[-\int_0^t P\left[\underline{k}(t')\right]dt'\right] dt \quad . \tag{2}$$

In principle if the distribution $P[\underline{k}(t)]$ is known then $P\,(t)$ may be calculated and a set of stochastic free flight times generated. However $P\,[\underline{k}(t)]$ is not a simple function and this would be a time consuming process. To avoid this problem we follow Rees(1969) and introduce the concept of self-scattering. We consider a fictitious scattering rate which complements the true scattering rate over the region of $\underline{k}$ space of interest, such that the total scattering rate,$\Gamma_0$, is a constant(see *Figure* 1),

$$P[\underline{k}(t)] = \Gamma_0 = \frac{1}{\tau_0} \ .$$

If the electron suffers a self-scattering event the momentum of the electron is unaltered. With this form for $\Gamma_0$ the integral in *equation* 2 is easily evaluated, hence

$$P\,(t) = \frac{1}{\tau_0} exp\left[-\frac{t}{\tau_0}\right] \ . \tag{3}$$

To generate a series of stochastic free-flight times we use the relation

$$r_1 = \int_0^{t_f} P\,(t)\,dt \ , \tag{4}$$

where we note $P\,(t)$ is normalised and $r_1$ is a random number evenly distributed on the range $[0, 1]$. Evaluating the integral we find

$$t_f = -\tau_0 \ ln(r_1) \ , \tag{5}$$

where we have used the nature of $r_1$. We see that it is now a simple operation to evaluate the free flight times.

The electron's new position and velocity just prior to scattering may easily be found by integrating,

$$m_e \frac{d\underline{v}}{dt} = -e(\underline{E} + \underline{v} \times \underline{B}) \ , \tag{6}$$

where $\underline{E}$ is the electric field which we assume is directed in the $z - direction$ and $\underline{B}$ is the magnetic field. We shall be concerned with the case when $\underline{B} = 0$. The integration of *equation* 6 is then particularly simple.

Once the new co-ordinates have been found the problem is to determine the type of scattering mechanism which the electron encounters and how the electron trajectory is altered.

# 3 The Scattering Event

## 3.1 Type of Mechanism

After the electron has travelled for the required free flight time a choice has to be made about how the electron scatters. We consider *figure* 1 which is a schematic diagram showing how the scattering rates vary as a function of electron speed and how self-scattering supplements the scattering rates over the

range of interest so that the total scattering rate is a constant. The electrons speed after the free-flight time fixes the type of scattering events which may participate and the rates at which they occur. To choose a particular mechanism we generate a random number evenly distributed on the range $[0, \Gamma_0]$, the mechanism is then selected by considering where this lies on *figure* 1. To determine the new trajectory we need to consider specific scattering mechanisms.

## 3.2 The New Trajectory

In the gas discharge problem there are two common types of electron number preserving scattering mechanism to consider, both of which relax energy. In both cases the electron is assumed to scatter isotropically off a gas molecule and the change in electron energy is dependent on the mechanism type. For recoil scattering the change in kinetic energy, $\Delta E$, is given by,

$$\Delta E = E_i \frac{2m_e}{M}(1 - \cos\gamma) \quad . \tag{7}$$

where $\gamma$ is the angle through which the electron is scattered, $m_e$ is the mass of the electron, $M$ is the mass of the gas molecule and $E_i$ is the energy just before the collision. The other energy relaxing process involves the excitation of a gas molecule. Hence,

$$\Delta E = E_{ex} \quad , \tag{8}$$

where $E_{ex}$ is an excitation energy. In calculating the new electron trajectory we fix the new direction of travel through the relations,

$$r_2 = (2\cos\phi - 1) \quad , \tag{9}$$

and

$$\theta = 2\pi r_3 \quad , \tag{10}$$

where $r_2$ and $r_3$ have the same properties as $r_1$. Equations 9 *and* 10 ensure that the scattering is isotropic. The new speed is then determined by evaluating the scattering angle and considering *equations* 7 *and* 8.

As well as the energy relaxing processes which conserve electron number it is possible for electrons to get trapped by the gas atoms (attachment) leading to a decay in electron numbers. The corresponding electron growth process is due to energetic electrons ionising the gas atoms. We assume that the electrons which attach are lost for all time. We also assume that after an ionising collision the primary and secondary electrons have the same kinetic energy.

The Monte-Carlo algorithm simply involves drifting a swarm of electrons for some simulation time and taking note of their positions and velocities at the end. It is then a simple matter to evaluate any distribution of interest. When the mean energy of the swarm has reached a steady state value we can drift the swarm for further short time steps. The electron distribution functions after each of the time steps can then be added together to give a smoother distribution. In this report our distributions were calculated for a swarm of $\approx 17000$ *electrons* monitored at 1000 *points*, so the resulting average histograms are the result of considering $\approx 1.7 \times 10^7$ *electrons*.

# 4 Results for Sulphur Hexa-Fluoride($SF_6$)

In this section we consider the behaviour of an electron swarm in Sulphur Hexa-Fluoride ($SF_6$). $SF_6$ is a chemically inert gas which is of practical importance in several areas. Its resistance to electrical breakdown makes it useful as an electrical insulator whilst its ability to trap electrons can be used to reduce the recovery time of high tension switch gear. $SF_6$ is also important as a chemical etchant in plasma etching systems where the $SF_6$ molecule is broken down by the application of a high voltage. This ability to donate fluorine atoms also makes $SF_6$ a useful constituent in chemical lasers.

Although the cross-sections for $SF_6$ have been well researched their exact form is still uncertain [see Itoh et al(1990) for a discussion]. We have taken the cross-sections used by Itoh(1988) and the form of the cross-sections is shown in *figure* 2. We considered an electric field to $SF_6$ number density ratio, $\frac{E}{N}$ value, of $367Td$ ($1Td \equiv 1 \times 10^{-21} Vm^2$). We released 17000 electrons with zero speed and we allowed them to drift through a gas of $SF_6$ molecules at a pressure of 0.3 *Torr* for $100ns$. The average energy of the swarm was monitored every $0.05ns$. After $50ns$ the electron energy distributions at each subsequent time step were added together to give a low noise steady state histogram(see *figure* 3). The smooth curve also shown in *figure* 3 is the result of solving the Boltzmann equation[Milsom(1990)] showing good agreement between the two.

The mean energy of the swarm of electrons as a function of time may be seen in *figure* 4 we see that it takes $\approx 15ns$ for the electron swarm to settle down to a steady state and this figure should scale roughly with the inverse of pressure for the same $\frac{E}{N}$ value, so high pressure gases should achieve the steady state very rapidly.

The electron speed distributions in the $x$, $y$ *and* $z$ directions were also calculated (see *figure* 5). We note that the x and y speed distributions are sym-

metric about the speed axis, whilst the z distribution is weighted in the direction of the applied electrostatic force, as expected. The electron growth/decay was also monitored and may be seen in *figure* 6 $hereE/N = 370Td$. The initial drop in electron number is due to low energy electrons attaching. The electrons which are lucky enough to escape this process are accelerated by the electric field and eventually have enough energy to avoid attachment. The tail of the curve is due to a steady state electron energy distribution. We varied the $\frac{E}{N}$ value and monitored the slope of this tail, a graph of electron growth rate against $\frac{E}{N}$ is shown in *figure* 7. The stable working field is when the two processes are balanced on refering to *figure* 7 we see this is at $\approx 367Td$.

# 5 Discussion

We have seen that it is a simple matter to obtain exact electron distribution functions for an electron swarm in a gas by using the Monte-Carlo method. This technique is computer time intensive and results can only be obtained on a reasonable time scale ($\approx$ *minutes*) if parallel computing methods are used. It took approximately 20 minutes to obtain a smooth electron distribution for an electron swarm in $SF_6$ using 17 *transputers*. The results for $SF_6$ compare favourably with the results of a Boltzmann analysis, giving confidence in both methods. However there are differences between the distributions. The Boltzmann analysis uses an approximate relaxation time and involves considering only the first two spherical harmonics of the electron distribution function, in view of this the overall agreement is pleasing.

We are also able to predict stable working fields to within a few percent and this should prove useful when we consider gas mixtures in the future.

# 6 Conclusions

A Monte-Carlo computer code has been written which can routinely predict the swarm parameters of electrons in a gas and stable working fields are also predicted. The electron energy distribution function derived from an analysis of the Boltzmann equation compares well with that from the Monte-Carlo, indicating that the two-term Boltzmann technique is useful for a quick assesment.

## Acknowledgements

I am indebted to Dr J.H.Jefferson for many helpful discussions and for suggesting the transputer method. I would also like to thank Mr. E.K.Gorton for bringing the problem to my attention.

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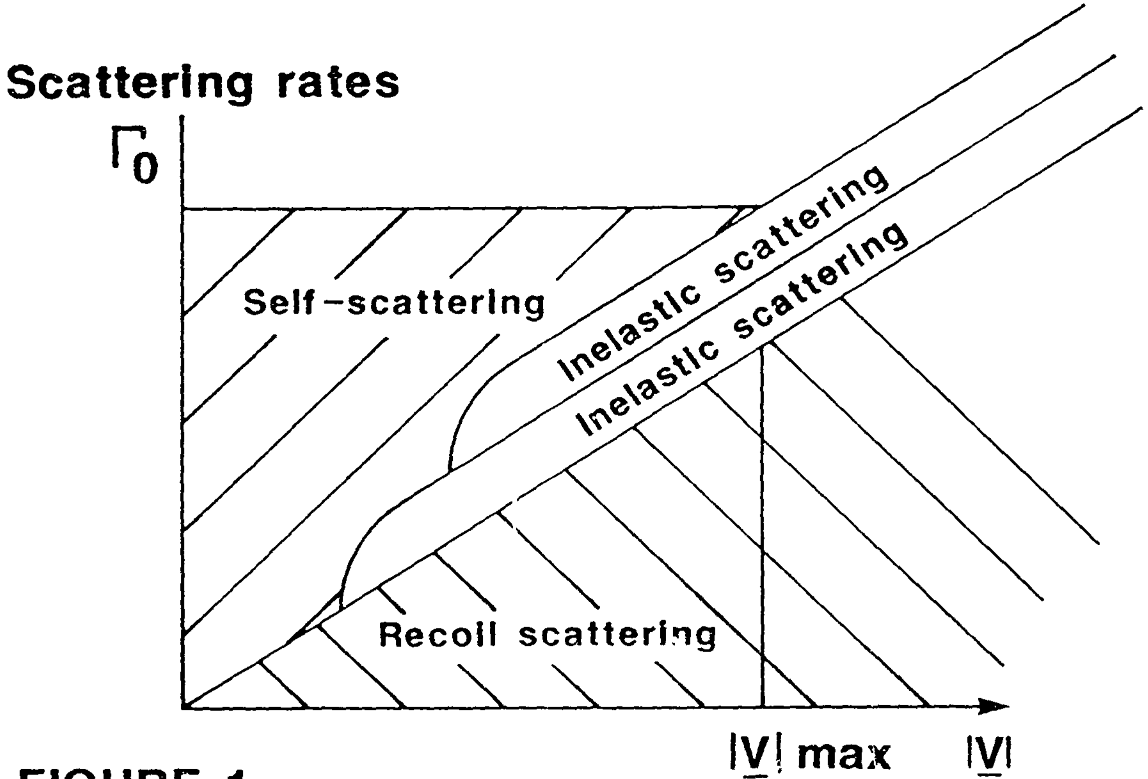



FIGURE 1

Individual and cumulative scattering rates showing how self-scattering complements the true scattering rate over the region of interest, so that the total scattering rate is a constant, $\Gamma_0$

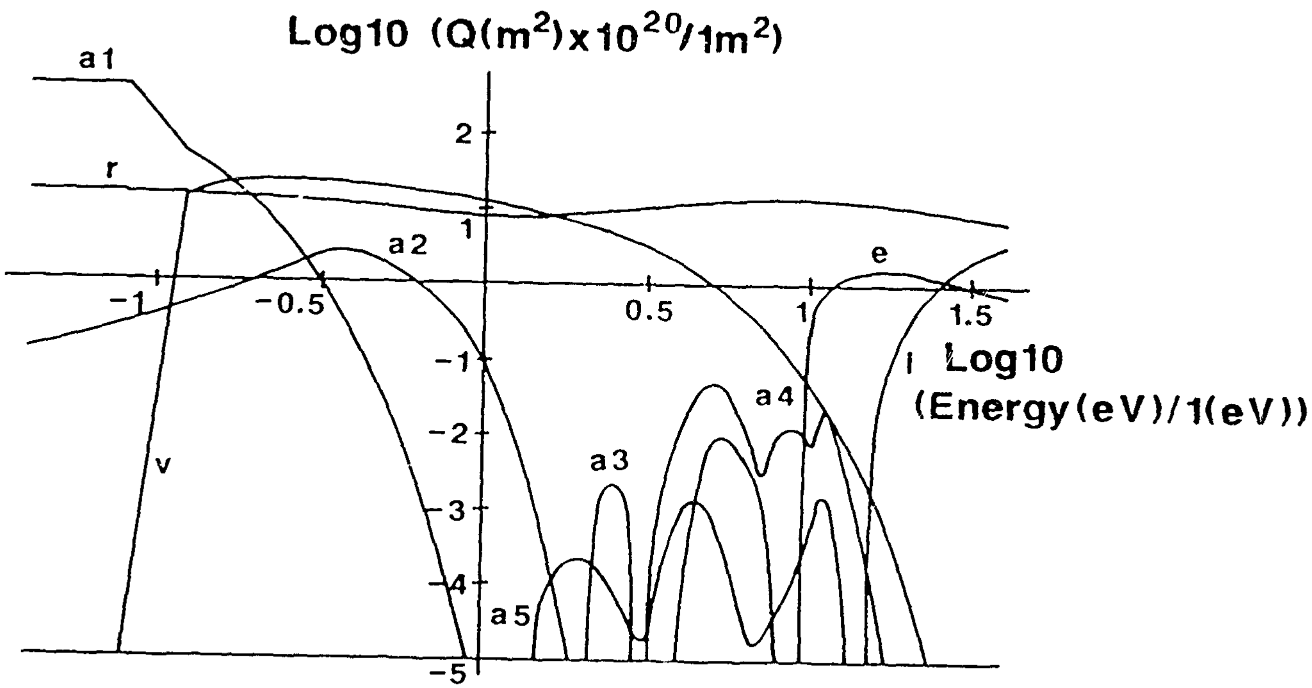



FIGURE 2

electron-$SF_6$ collision cross-sections on log/log scales.

r=recoil cross-section

v=a vibrational excitation cross-section

e=an electronic excitation cross-section

a=an attachment cross-section

i=an ionisation cross-section

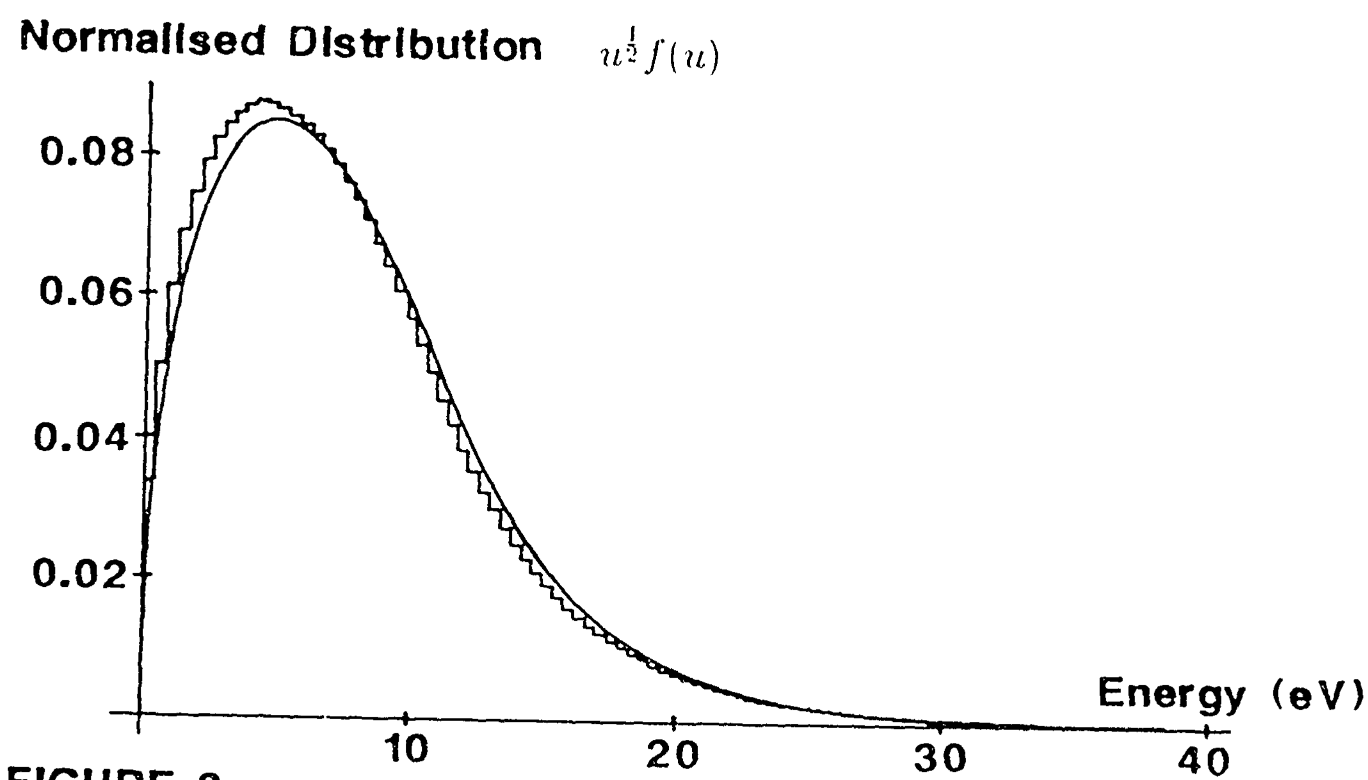



FIGURE 3

Steady-state electron energy distribution functions.
The Histogram is the result of a Monte-Carlo Simulation, whilst the curve results from solving the Boltzmann equation.
($E/N$ =367Td)

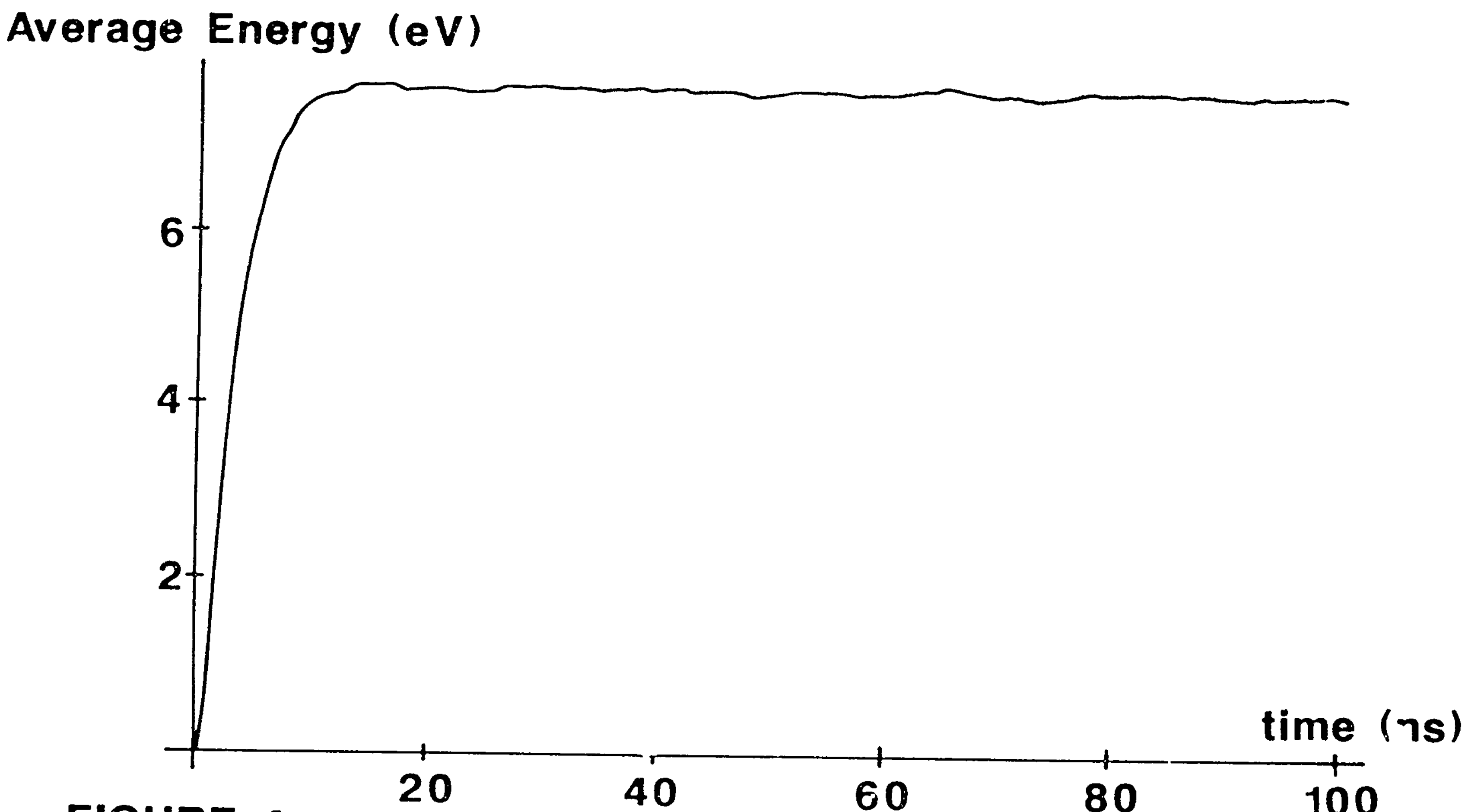



FIGURE 4

The average energy of the electron swarm as a function of time showing the approach to the steady state.

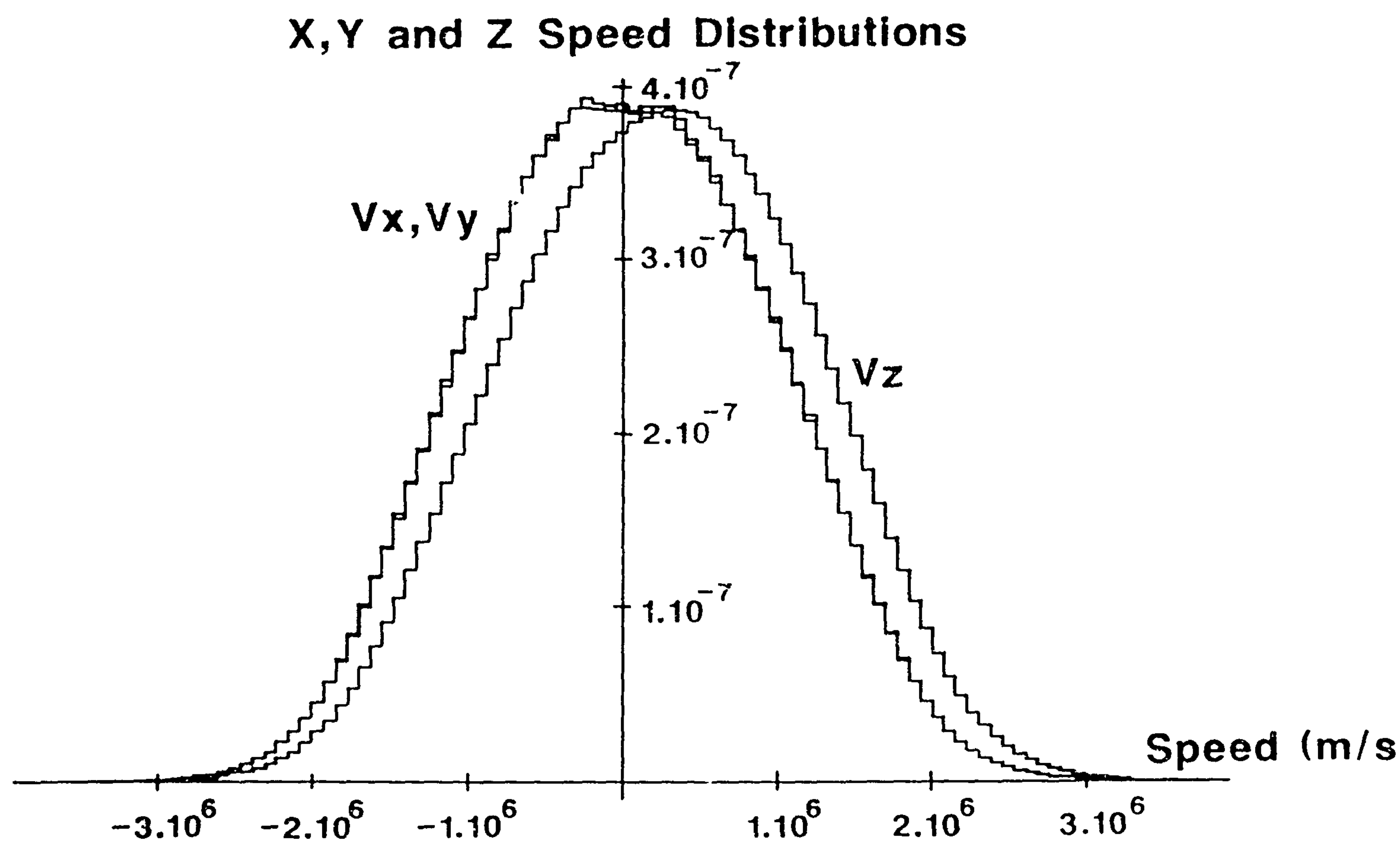



FIGURE 5

Normalised steady-state speed distributions. The assymmetry of the Vz distribution is due to the application of the electric field.

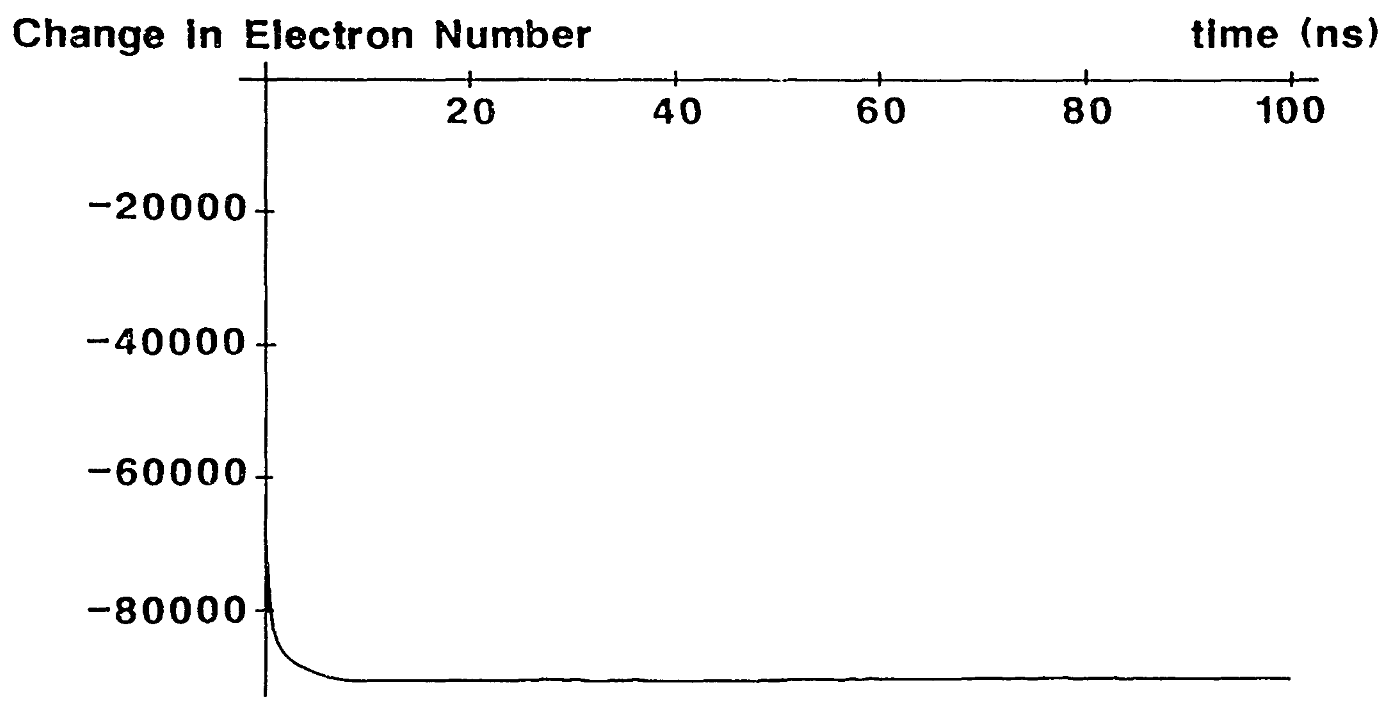
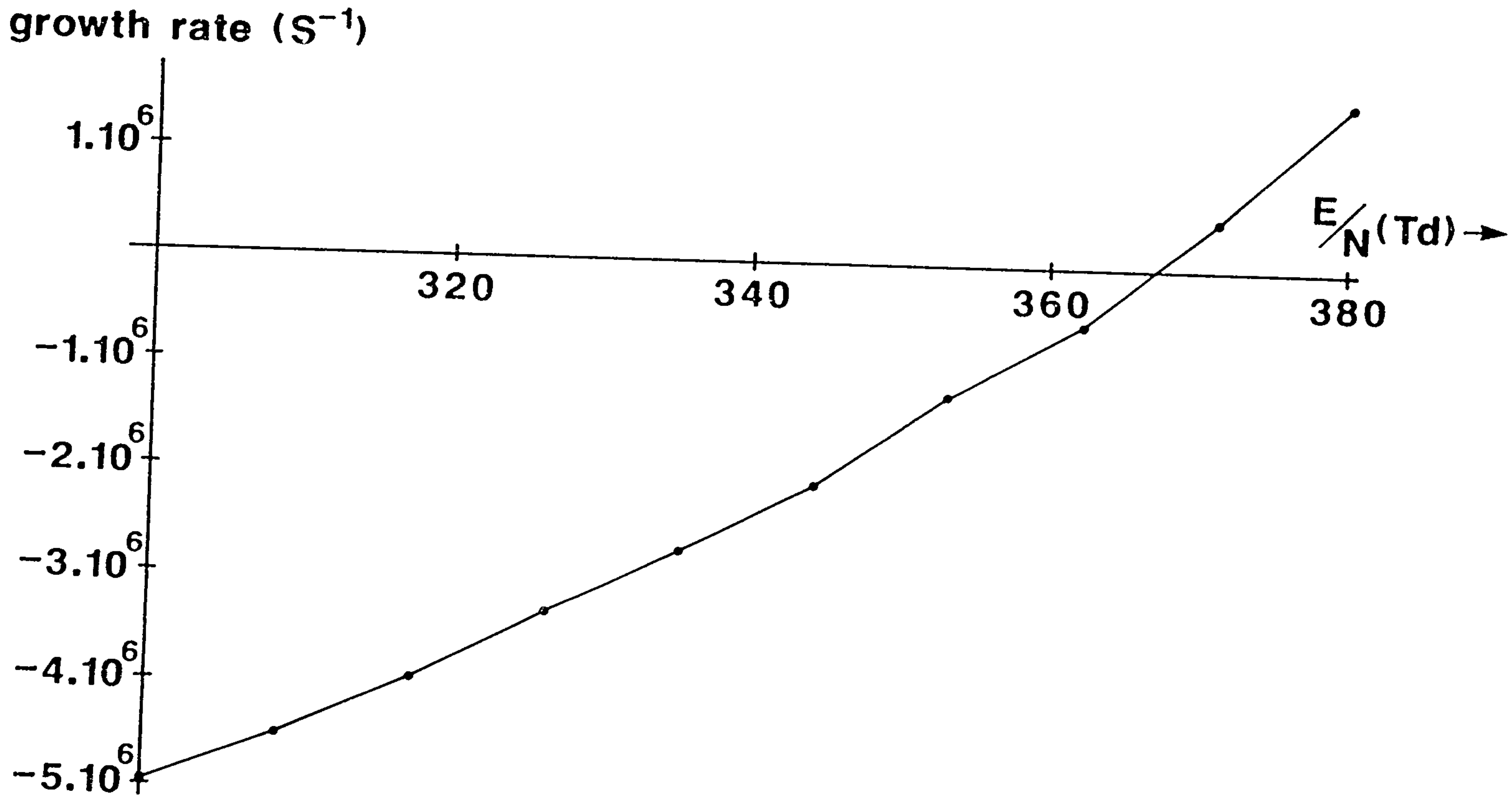



FIGURE 6

The graph shows the rapid decrease in electron numbers due to the attachment process. Electrons lucky enough to avoid this process for the first 15ns are unlikely to attach.




## FIGURE 7

The Electron growth rate as a function of $E/N$. The intersection with the axis indicates the stable working field which is around 365Td.

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Abstract

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